

# Pauli equations and non-commutative position operators in 2D Dirac-like semiconductors in view of second quantization

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The Pauli equations describing electron (hole) dynamics in 2D Dirac-like intrinsic semiconductors in external (impurity) scalar potential and for inhomogeneous lattice distortions are obtained within second quantization approach. We show that the modifying external perturbation terms in formulated no-pair equations are in general non-local and demonstrates singular behavior in gapless situation where they do not depend on semiconductor parameters. It is shown that lattice distortion perturbation can cause confinement of both electrons and holes in the same spatial region. The proposed approach is verified by comparison with well-established results in low energy limit. The consideration of position operator in second quantization approach allows elucidating the physical meaning of spin-orbit-like and Darwin-like terms.

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## I. INTRODUCTION

The Pauli single particle equations (SPE) emerge in atomic physics as a non-relativistic approximation to the “exact” relativistic Dirac equation. The truncated  $2 \times 2$  Hamiltonian describes only electrons or positrons (holes). In obtained Schrodinger-like equation the external potential (in atomic physics the potential of nucleus) is modified. The famous term known as spin-orbit interaction (SOI):  $\frac{\hbar}{4m_0^2c^2} \boldsymbol{\sigma} [\nabla V(r) \times \hat{\mathbf{p}}]$  is added to bare potential. The inclusion of this term is necessary for correspondence of theoretical results with experimental data [1]. The problem of reduction of multicomponent relativistic problem constructing approximate quasi-relativistic two component Hamiltonian has been and is under intensive discussion in low and intermediate nuclear physics and in molecule physics for heavy-atom species. It is the long established fact that “quasi-relativistic” problems infest any multiband semiconductor  $\mathbf{k} \cdot \mathbf{p}$  Hamiltonians [2, 3]. The band structure of semiconductors described in  $\mathbf{k} \cdot \mathbf{p}$  theory by matrix Hamiltonians takes into account at least two (electron and hole-like) bands. Such Dirac-like artifacts as constant carrier velocity and Zitterbewegung emerge if we proceed along the “classical” line of approach, allowing for interference of positive and negative states [4]. The Klein paradox unimpeded penetration of carriers through high potential barrier, emerges as an essential attribute of graphene physics described within gapless Dirac-like Hamiltonian [5]. According to seminal paper by Keldysh [6] the problem of supercharged nuclei transforms in semiconductors into the problem of deep levels of impurity centers. Thus, the problem of reduction of generic multicomponent Hamiltonians, which not only makes the computation feasible but elucidates the underlying physics, emerges as the interdisciplinary problem.

The standard derivation of Pauli SPE in Dirac theory follows two main approaches. The first approach is the construction of appropriate unitary transformation decoupling positive and negative modes of Dirac equa-

tion. The main schemes are famous Foldy-Wouthuysen (FW) transformation and its variant proposed by Erikssen, Douglas-Kroll-Hess approach [7–15]. The truncated Hamiltonian even in the lowest in  $c^{-1}$  order suffers from such drawbacks as lack of uniqueness and difficulties in obtaining higher order terms especially, if external potential is applied. It has no well-behaved wave functions and only expectation values obtained with these functions have physical meaning [10]. The analog of this approach is used for constructing reduced  $\mathbf{k} \cdot \mathbf{p}$  Hamiltonians for degenerate spectrum [16]. The second approach is the Pauli subtraction method (small component method) which eliminates two components, considered to be small, from the four-component wave function [17, 18]. Within this method block-diagonal energy-dependent Hamiltonians are constructed. Under this transformation non-Hermitian terms may appear [14]. Known as Lowdin partitioning [19], this approach is used usually for reduction of multicomponent  $\mathbf{k} \cdot \mathbf{p}$  Hamiltonians.

The commonly accepted point of view is that Dirac equation is not the single particle equation. Rigorously, the Dirac equation is self-consistent only in the context of quantum field theory (QFT), especially if external potential is applied. This is due to nonzero probability of particle-antiparticle creation/annihilation. The space-time resolved solutions to relativistic QFT allows to clarify the physics of Klein paradox and Zitterbewegung effect [20, 21]

Bearing in mind discussed above quasi-relativistic similarity of the problems arising in  $\mathbf{k} \cdot \mathbf{p}$  description, we approach the problem of formulation of Pauli electron(hole)-only equations in the theory with external perturbations from the point of QFT using the second quantization method (SQM). The account for filled valence band allows us to use electron-hole semiconductor language as the quantum number “charge” is ascribed to the eigenfunctions of appropriate reduced two-component Pauli Hamiltonians. As pointed by Feynman “The problem of charges in a fixed potential is usually treated by the method of second quantization of electron

field, using the ideas of the theory of holes" [22].

Note that the second quantization prohibits in general the direct probabilistic interpretation of the field operators, as compared to commonly used quantum mechanical wave functions [23]. The superposition of the states with variable number of particles is not compatible with the simple interpretation of wave function. Moreover the possible interpretation crucially depends on the choice of single particle projection space [23].

In this paper the sought SPE are obtained neglecting pair creation processes (stability of vacuum under external perturbation) so they are logically to be called as "no-pair equations". The decoupling of electrons and holes degrees of freedom enables us to write down the Pauli-like equations for each of these carriers separately.

The paper is organized as follows. In Sec. II, we obtain single particle Pauli equations for 2D Dirac-like semiconductor and compare our results with well-established ones. In Sec. III, we analyze properties of the position operator and its connection with spin-orbit-like and Darwin-like terms.

## II. PAULI EQUATIONS IN 2D DIRAC-LIKE SEMICONDUCTOR

Leaving aside pure relativistic problems Dirac Hamiltonian is considered as an example of effective  $\mathbf{k} \cdot \mathbf{p}$  Hamiltonian, describing two-band semiconductor with symmetrical conduction and valence bands. The Dirac Hamiltonian has the following form

$$\hat{H}_D = \begin{pmatrix} \frac{E_g}{2} & 0 & \gamma k_z & \gamma k_- \\ 0 & \frac{E_g}{2} & \gamma k_+ & -\gamma k_z \\ \gamma k_z & \gamma k_- & -\frac{E_g}{2} & 0 \\ \gamma k_+ & -\gamma k_z & 0 & -\frac{E_g}{2} \end{pmatrix}, \quad (1)$$

where  $k_{\pm} = k_x \pm ik_y = ke^{\pm i\varphi(\mathbf{k})}$ ,  $\gamma$  - characteristic velocity,  $E_g$  - energy gap. In relativistic Dirac theory  $E_g = 2mc^2$  and  $\gamma = c$ . Here and in the following  $\hbar = 1$ .

To simplify the following analysis, we consider 2D version of Hamiltonian (1). Choosing  $k_z = 0$  two groups of states ( $e \ 1/2, h \ -1/2$ ) and ( $e \ -1/2, h \ 1/2$ ) do not mix. The Hamiltonian for the former group of these states reads

$$\hat{H}_D = \begin{pmatrix} \frac{E_g}{2} & \gamma k_- \\ \gamma k_+ & -\frac{E_g}{2} \end{pmatrix}. \quad (2)$$

The Hamiltonian matrix for the second group of states is obtained by replacing  $k_y$  by  $-k_y$ . In this section we consider only first group of states described by Hamiltonian (2). The energy eigenvalues of (2) are

$$\varepsilon(k)_{1,2} = \pm \sqrt{\frac{E_g^2}{4} + \gamma^2 k^2} \equiv \pm \varepsilon(k). \quad (3)$$

The electrons and holes eigenstates are chosen as

$$\varphi_e(\mathbf{k}) = \begin{pmatrix} \cos \Theta(\mathbf{k}) \\ \sin \Theta(\mathbf{k}) e^{i\varphi(\mathbf{k})} \end{pmatrix}, \quad (4)$$

$$\varphi_h(\mathbf{k}) = \begin{pmatrix} -\sin \Theta(\mathbf{k}) e^{-i\varphi(\mathbf{k})} \\ \cos \Theta(\mathbf{k}) \end{pmatrix}, \quad (5)$$

where

$$\cos \Theta(\mathbf{k}) = \frac{\sqrt{\varepsilon(k) + E_g/2}}{\sqrt{2\varepsilon(k)}}, \quad (6)$$

$$\sin \Theta(\mathbf{k}) = \frac{\sqrt{\varepsilon(k) - E_g/2}}{\sqrt{2\varepsilon(k)}}. \quad (7)$$

In the special case  $E_g = 0$  Hamiltonian (2) is used for the description of electrons in  $K$  valley in graphene

$$\hat{H}_K = \gamma \begin{pmatrix} 0 & k_- \\ k_+ & 0 \end{pmatrix}. \quad (8)$$

In this case we are dealing with pseudospin, which is a formal way of taking into account the two carbon atoms per unit cell [24], and the quasi-momentum  $k$  is measured from Dirac points. In the second quantization picture the Hamiltonian (2) for intrinsic semiconductor is

$$\hat{H}_D = \int \varepsilon(k) \hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{k}) \frac{d\mathbf{k}}{(2\pi)^2} + \int \varepsilon(k) \hat{b}^\dagger(\mathbf{k}) \hat{b}(\mathbf{k}) \frac{d\mathbf{k}}{(2\pi)^2}. \quad (9)$$

Here  $\hat{a}^\dagger(\mathbf{k})$ ,  $\hat{a}(\mathbf{k})$  are creation/annihilation operators for electrons and  $\hat{b}^\dagger(\mathbf{k})$ ,  $\hat{b}(\mathbf{k})$  are corresponding operators for holes. Inserting the potential  $V(\mathbf{r})$  into empty Hamiltonian diagonal we obtain the following additional terms in the Hamiltonian

$$\begin{aligned} \hat{H}_i = & \int \int \varphi_e^*(\mathbf{k}) \varphi_e(\mathbf{q}) V(\mathbf{k} - \mathbf{q}) \hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{q}) \frac{d\mathbf{k} d\mathbf{q}}{(2\pi)^4} \\ & - \int \int \varphi_h^*(\mathbf{k}) \varphi_h(\mathbf{q}) V(\mathbf{k} - \mathbf{q}) \hat{b}^\dagger(-\mathbf{q}) \hat{b}(-\mathbf{k}) \frac{d\mathbf{k} d\mathbf{q}}{(2\pi)^4} \\ & + \int \int \varphi_e^*(\mathbf{k}) \varphi_h(\mathbf{q}) V(\mathbf{k} - \mathbf{q}) \hat{a}^\dagger(\mathbf{k}) \hat{b}^\dagger(-\mathbf{q}) \frac{d\mathbf{k} d\mathbf{q}}{(2\pi)^4} \\ & + \int \int \varphi_h^*(\mathbf{k}) \varphi_e(\mathbf{q}) V(\mathbf{k} - \mathbf{q}) \hat{b}(-\mathbf{k}) \hat{a}(\mathbf{q}) \frac{d\mathbf{k} d\mathbf{q}}{(2\pi)^4}. \end{aligned} \quad (10)$$

The terms containing  $\hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{q})$  and  $\hat{b}^\dagger(\mathbf{q}) \hat{b}(\mathbf{k})$  describe the processes of scattering electrons/holes by the potential modified by the presence of filled valence band. The terms containing  $\hat{a}^\dagger(\mathbf{k}) \hat{b}^\dagger(-\mathbf{q})$  and  $\hat{b}(-\mathbf{k}) \hat{a}(\mathbf{q})$  describe the perturbation of vacuum (filled valence band) As it seen the second quantization version of considered Dirac Hamiltonian is a many-particle Hamiltonian due to possibility of electron-hole pairs creation and annihilation by external potential, even when inter-particle interaction (as in our work) is not accounted for. Note, that under the term "external" potential we understood not only external action but internal action due to impurities

as well.

The explicit expression for modified no-pair electron scattering potential is

$$V_e = \int \int \left( \cos \Theta(\mathbf{k}) \cos \Theta(\mathbf{q}) + \sin \Theta(\mathbf{k}) \sin \Theta(\mathbf{q}) e^{-i\Delta(\mathbf{k}, \mathbf{q})} \right) \times V(\mathbf{k} - \mathbf{q}) \hat{a}^+(\mathbf{k}) \hat{a}(\mathbf{q}) \frac{d\mathbf{k}}{(2\pi)^2} \frac{d\mathbf{q}}{(2\pi)^2}, \quad (11)$$

where  $\Delta(\mathbf{k}, \mathbf{q}) = \varphi(\mathbf{k}) - \varphi(\mathbf{q})$ . The expression for holes (positrons) is of the same functional form but has opposite sign.

Finally, the spectrum for single particle electron problem is derived from Heisenberg equation of motion

$$\frac{d\hat{a}}{dt} = i [H_p, \hat{a}(\mathbf{k})],$$

where single particle no-pair Pauli Hamiltonian  $H_p$  for electron runs as follows:

$$H_p = \int \varepsilon(\mathbf{k}) \hat{a}^+(\mathbf{k}) \hat{a}(\mathbf{k}) \frac{d\mathbf{k}}{(2\pi)^2} + V_e, \quad (12)$$

where  $\varepsilon(\mathbf{k})$  and  $V_e$  are given by the formulas (3) and (11), respectively. The solution of Heisenberg equation is given by the solution of Eigen problem of corresponding no-pair Pauli-type equation:

$$E \varphi(\mathbf{k}) = \varepsilon(\mathbf{k}) \varphi(\mathbf{k}) + \int \left( \cos \Theta(\mathbf{k}) \cos \Theta(\mathbf{q}) + \sin \Theta(\mathbf{k}) \sin \Theta(\mathbf{q}) e^{-i\Delta(\mathbf{k}, \mathbf{q})} \right) \times V(\mathbf{k} - \mathbf{q}) \varphi(\mathbf{q}) \frac{d\mathbf{q}}{(2\pi)^2}. \quad (13)$$

Modified electron scattering potential (13) loses its translational invariance in momentum space and as a corollary becomes non-local in coordinate representation. The obtained equation coincides conceptually with the no-pair equation derived in [25] for hydrogenic systems within quantum electrodynamic (QED), allowing to make rigorous reduction into the system that contains a single electron but no positrons. The analogous no-pair equations has been derived with free particle projection operators for atomic orbital calculations on one-electron atoms [9].

As it was pointed out, the Pauli-like equation for holes differs from (13) by sign. It means that potential perturbation inserted into diagonal of  $\mathbf{k} \cdot \mathbf{p}$  Hamiltonian (even when its “electro-magnetic” nature is not specialized) discriminates between particle charges. Thus, if it is attractive for electrons, it is repulsive for holes and vice versa. The account for omitted pair production terms up to the second order in  $V(k)$  will lead to the appearance of the terms proportional to square of potential, which are charge insensitive and act on electrons and holes alike. In this approximation the solutions of obtained equation will predict the same effects as the equation proposed by L.Keldysh [6] for the description of deep levels.

The simultaneous confinement of electrons and holes

within proposed approach can occur only due to spatial dependence of band gap (mass term in Dirac equation). Following [26] we account for smooth inhomogeneous lattice distortion by varying band gap:  $E_g \rightarrow E_{g0} + \delta E_g(\mathbf{r})$ . As a result the following additional terms in no-pair equations for electrons and holes appear respectively

$$\frac{1}{2} \int \int \left( \cos \Theta(\mathbf{k}) \cos \Theta(\mathbf{q}) + \sin \Theta(\mathbf{k}) \sin \Theta(\mathbf{q}) e^{-i\Delta(\mathbf{k}, \mathbf{q})} \right) \times \delta E_g(\mathbf{k} - \mathbf{q}) \hat{a}^+(\mathbf{k}) \hat{a}(\mathbf{q}) \frac{d\mathbf{k}}{(2\pi)^2} \frac{d\mathbf{q}}{(2\pi)^2}, \quad (14)$$

$$\frac{1}{2} \int \int \left( \cos \Theta(\mathbf{k}) \cos \Theta(\mathbf{q}) - \sin \Theta(\mathbf{k}) \sin \Theta(\mathbf{q}) e^{i\Delta(\mathbf{k}, \mathbf{q})} \right) \times \delta E_g(\mathbf{k} - \mathbf{q}) \hat{b}^+(\mathbf{k}) \hat{b}(\mathbf{q}) \frac{d\mathbf{k}}{(2\pi)^2} \frac{d\mathbf{q}}{(2\pi)^2}. \quad (15)$$

Contrary to the statement in [26] this perturbation cannot be identified as some electric field. In contrast, the signs for such “mass” perturbation do not depend on quasi-particle charge and are the same for electrons and holes. It means that if confinement occurs for electrons due to proposed mechanism, the holes can localize within the same space region. The position dependence of band edges and effective masses were originally incorporated into  $\mathbf{k} \cdot \mathbf{p}$ -type analysis for calculation of band structure of GaAs-GaAlAs and InAs-GaSb superlattices in [27]. The necessity of the presence of band inversion or mass domain walls for the occurrence of localized edge states in graphene was underlined in [28–30].

If equation (13) is rewritten in a coordinate representation, the potential  $V_e$  becomes non-local. Thus instead of obtaining differential Schrodinger-type of equation we are to consider integro-differential one. Nevertheless, it is possible to hide this smearing of potential and reduce this equation to the well-known form used in atomic physics where SOI emerges. This is achieved by the expansion of  $H_p$  including the terms up to the second order in parameter  $\gamma k/E_g$ . Within this approximation the kinetic part becomes  $\varepsilon(k) \approx E_g/2 + \gamma^2 k^2/E_g - \gamma^4 k^4/E_g^3$  and  $V_e$  can be presented as the sum of two terms: “bare” potential and additional term:

$$V_e \approx \int \int V(\mathbf{k} - \mathbf{q}) \hat{a}^+(\mathbf{k}) \hat{a}(\mathbf{q}) d\mathbf{k} d\mathbf{q} - \frac{\gamma^2}{2E_g^2} \int \int \{2i[\mathbf{k} \times \mathbf{q}]_z - (\mathbf{k} - \mathbf{q})^2\} \times V(\mathbf{k} - \mathbf{q}) \hat{a}^+(\mathbf{k}) \hat{a}(\mathbf{q}) \frac{d\mathbf{k}}{(2\pi)^2} \frac{d\mathbf{q}}{(2\pi)^2}. \quad (16)$$

The inequality  $\gamma k/E_g \ll 1$  has simple physical meaning: the characteristic “Compton” wavelength  $\lambda_C = \gamma/E_g$  is small as compared with the characteristic length of spatial variation of electron/hole envelope function  $\lambda = 1/k$ . The condition  $\lambda_C \ll \lambda$  is always implied while considering semiconductors problems within envelope function approximation (EFA). The corresponding to (16) equation for electron Eigen functions (compare with (13)) is

a familiar expression with SOI and Darwin terms modifying external potential.

$$\left(E - \frac{E_g}{2}\right) \varphi(\mathbf{r}) = \left[\frac{\gamma^2 p^2}{E_g} - \frac{\gamma^4 p^4}{E_g^3}\right] \varphi(\mathbf{r}) + \left\{V(\mathbf{r}) + \frac{\gamma^2}{E_g^2} [\nabla V(\mathbf{r}) \times \mathbf{p}]_z + \frac{\gamma^2}{2E_g^2} \nabla^2 V(\mathbf{r})\right\} \varphi(\mathbf{r}) \quad (17)$$

This correspondence with well known, if trivial result, is presented only for validation of consideration proposed which we are going to apply elsewhere to more sophisticated  $\mathbf{k} \cdot \mathbf{p}$  Hamiltonians.

It is interesting to compare the additional terms induced by scalar potential and lattice distortions (spatially dependent band gap) in considered Pauli no-pair equations. In order to make our point more clearly let us consider 1D variant of considered problem with  $k_y = 0$  in low energy range (EFA). In this case only Darwin term survives in the expression for modified scalar potential

$$- \int (k_x - q_x)^2 V(k_x - q_x) \hat{a}^+(k_x) \hat{a}(q_x) \frac{dk_x}{2\pi} \frac{dq_x}{2\pi}. \quad (18)$$

Lattice distortion induces the following term

$$- \int (k_x + q_x)^2 \delta E_g(k_x - q_x) \hat{a}^+(k_x) \hat{a}(q_x) \frac{dk_x}{2\pi} \frac{dq_x}{2\pi}. \quad (19)$$

The difference in sign has far-reaching consequences. In the corresponding Schrodinger-like equation in coordinate space the modifying term for scalar potential is  $V_x''(x)\varphi(x)$ . The band gap variation induces additional terms

$$-\delta E_g''(x)\varphi(x) - 4\delta E_g'(x)\varphi'(x) - 4\delta E_g(x)\varphi''(x). \quad (20)$$

At first glance, this expression looks very strange if not to remember that in  $\mathbf{k} \cdot \mathbf{p}$  theory the energy gap determines such important characteristic as effective mass  $m^*$  around conduction (valence) band minimum (maximum). In our Dirac problem effective mass is  $m^* = E_{g0}/2\gamma^2$ . In classical theory the kinetic term with spatially dependent mass is  $-p^2 \delta m(r)/2(m_0^*)^2$ . In quantum theory the appearance of  $\mathbf{r}$  dependent mass in kinetic term poses the problem of appropriate ordering prescription. The best known procedure coping with this arbitrariness in Hamiltonian definition has been proposed by Weyl [31]. For a product of operators  $\{\hat{Q}_1 \dots \hat{Q}_n\}$  the Weyl ordering is defined as the sum over all permutations  $P(i_1 \dots i_n)$  of the indices. For the product of  $p^2$  and  $r$  it prescribes the use of the operator  $(p^2 r + 2prp + rp^2)/4$ . It is easy to verify, that in our approach this problem is solved in the favor of of such ordering

$$-\frac{1}{4} \left( \hat{p}^2 \frac{\delta m(r)}{2(m_0^*)^2} + \frac{\delta m(r)}{2(m_0^*)^2} \hat{p}^2 + 2\hat{p} \frac{\delta m(r)}{2(m_0^*)^2} \hat{p} \right). \quad (21)$$

The necessity of application of Weyl ordering in mathematically similar problems has been considered in [32–34]. As it was pointed in [35], in the FW transformed Dirac-Pauli equations the “operators orderings is a matter of further investigations and particularly, considerable insight might be obtained by exploiting the analogy to the model of semiconductor heterostructures”.

One additional remark is necessary. As follows from above there are no any ordering problems as long as our consideration is carried out within momentum space. All problems arise in the configurational space. It is one more advantage of this representation showed up in the cause of proposed approach to the reduction of multicomponent  $\mathbf{k} \cdot \mathbf{p}$  Hamiltonians. This contradicts the statement in [36] that reference to momentum space is “myth”. Using just this representation, we can bypass not only the ordering problem but can “consider the boundary conditions at interfaces in a natural way, and avoid automatically any spurious solutions” in quite general Hamiltonian as it has been argued in [37].

In the special case  $E_g = 0$  (graphene) external potential has rather simple form for electrons in no-pair approximation

$$V_e = \frac{1}{2} \int \int \left(1 + e^{-i\Delta(\mathbf{k}, \mathbf{q})}\right) V(\mathbf{k} - \mathbf{q}) \hat{a}^+(\mathbf{k}) \hat{a}(\mathbf{q}) \frac{d\mathbf{k} d\mathbf{q}}{(2\pi)^4}. \quad (22)$$

It is seen that the terms modifying scattering potential in the single particle channel are of the order of bare potential and do not depend on semiconductor parameters. Thus, generally their effect cannot be considered as perturbation even in single particle channel. One of the consequences is, that in the single particle scattering channel (as for electrons, so for holes) the back-scattering processes ( $\Delta(\mathbf{k}, \mathbf{q}) = \pi$ ) are strictly suppressed. The modified Pauli potential  $V_e \equiv 0$  for any chosen external scalar potential in this case. Here we have also correspondence with a well-known result in graphene physics, which is the origin of arising of topologically protected surface states [38, 39]. The most vivid example of this effect according to formulated equations is electron kinetics in 1D ( $k_y = 0$ ). As in this case  $\Delta(k_x, q_x)$  takes the 0,  $\pi$  values only, the interaction with impurity (external) potential is

$$V_e = \int \int (\Theta(k_x)\Theta(q_x) + \Theta(-k_x)\Theta(-q_x)) \times V(k_x - q_x) \hat{a}^+(k_x) \hat{a}(q_x) \frac{dk_x dq_x}{(2\pi)^2}, \quad (23)$$

where  $\Theta(x)$  is a Heaviside step function. It is seen that in the electron single particle channel in 1D problem we have independent “right” moving solutions spanned by  $\Theta(k_x)\hat{a}(k_x)$  the and “left” moving solutions formed by  $\Theta(-k_x)\hat{a}(k_x)$ . Note, that within considered approach this result holds as long as we do not take into account pair contribution. If particle number is not conserved, which means the admixture of the states “particle + pairs”, this restriction can be removed, leading to Andreev-like multi-particle type of reflection [40].

The effect of mass domain wall is also best demonstrated for  $E_{g0} = 0$  in 1D. (For example, this situation can be considered as the boundary of heterostructure CdTe/HgTe). In this case  $\Delta(\mathbf{k}, \mathbf{q}) = 0, \pi$  and the corresponding interaction is given by

$$V_e = \int \int (\Theta(k_x)\Theta(-q_x) + \Theta(-k_x)\Theta(q_x)) \times \delta E_g(k_x - q_x) \hat{a}^+(k_x) \hat{a}(q_x) \frac{dk_x dq_x}{(2\pi)^2}. \quad (24)$$

The same expression is valid for holes. As compare with potential scattering (23), lattice distortion favors back scattering and thus can lead to localization at such boundary as for electrons, so for holes.

Returning to the effect of potential modification in graphene, we must add that the noted possible spatial separation of electrons and holes by applied external perturbation is in accord with the results of [41]. In this paper the authors reported a new technique of Dirac point mapping of charge inhomogeneities in graphene. Using it, they have revealed that charge puddles are caused by charge-donating impurities below the graphene. At the same time they have ruled out the hypothesis that topographic corrugations in graphene were a primary cause of the charge separation. This result is also in accord with our conclusion that the effect of lattice distortions upon electrons and holes is alike.

To investigate further properties of modified potential in no-pair equations let us write it down for the linear potential  $V(\mathbf{r}) = F \cdot x$  chosen in momentum representation as

$$V(\mathbf{k} - \mathbf{q}) = F \cdot \frac{i}{2} \{ \delta'_{k_x}(\mathbf{k} - \mathbf{q}) - \delta'_{q_x}(\mathbf{q} - \mathbf{k}) \} \quad (25)$$

$$= F \cdot \delta'_{k_x, q_x}(\mathbf{k}, \mathbf{q}). \quad (26)$$

Substituting (25) into (11) we obtain two terms: one “trivial” term  $iF \frac{\partial}{\partial k_x} \varphi(k)$  describing interaction with “bare” potential and terms depending only on momentums which can be attributed to kinetic energy. The modified effective kinetic term in this case is

$$E_{kin,eff} = \varepsilon(\mathbf{k}) \pm F \frac{\gamma^2 k_y}{\varepsilon(k)(E_g + 2\varepsilon(k))} = \varepsilon(\mathbf{k}) \pm \frac{1}{2} F \frac{\partial}{\partial k_y} \ln(1 + 2\varepsilon(\mathbf{k})/E_g). \quad (27)$$

The different signs refer to two group of states of the problem. It follows from (27) that in EFA this expression acquires the customary Rashba form [42]

$$E_{kin,eff} \approx \frac{\gamma^2 k^2}{E_g} \pm \frac{F\gamma^2}{E_g^2} k_y, \quad (28)$$

where  $F\gamma^2/E_g^2$  plays the role of effective Rashba coupling constant.

If the electric field is applied along Y axis the Rashba

term will be

$$\mp \frac{1}{2} F \frac{\partial}{\partial k_x} \ln(1 + 2\varepsilon(\mathbf{k})/E_g). \quad (29)$$

Thus in considered approach Rashba effect can be considered as due to some Berry-like field acting in momentum space with connection

$$\mathbf{A}(\mathbf{k}) = (\gamma^2 k_x / f(k), -\gamma^2 k_y / f(k)), \quad (30)$$

where  $f(k) = \varepsilon(k)(E_g + 2\varepsilon(k))$ . The corresponding Berry-like curvature has the most simple form in EFA

$$\Omega_z \approx \frac{\gamma^2}{E_g^2} = \lambda_C^2. \quad (31)$$

The statement that arising of Rashba term is due to Berry-like field will be confirmed additionally below while considering position operator within SQM.

### III. POSITION OPERATOR IN 2D DIRAC-LIKE SEMICONDUCTOR

Let us consider obtained results from another point of view. We will be interested in the form and properties of position operator  $\hat{\mathbf{r}}$  in SQM. Using the definition

$$\begin{aligned} \hat{\mathbf{r}} &= \sum_{s=1,2} \int \int \Psi_s^+(\mathbf{k}) \delta'_{k_x, q_x}(\mathbf{k}, \mathbf{q}) \Psi_s(\mathbf{q}) \frac{d\mathbf{k}}{(2\pi)^2} \frac{d\mathbf{q}}{(2\pi)^2} \\ &= \sum_{s=1,2} \int \hat{\mathbf{r}}_s(\mathbf{k}) \frac{d\mathbf{k}}{(2\pi)^2}, \end{aligned} \quad (32)$$

we obtain

$$\hat{\mathbf{r}}(\mathbf{k}) = \sum_{s=1,2} \left( \hat{\mathbf{R}}_s(\mathbf{k}) + \hat{\mathbf{A}}_s(\mathbf{k}) + \hat{\mathbf{B}}_s(\mathbf{k}) \right). \quad (33)$$

Here

$$\hat{\mathbf{R}}_s(\mathbf{k}) = \hat{\mathbf{r}}_{Sch}(\mathbf{k}) \left( \hat{a}_s^+(\mathbf{k}) \hat{a}_s(\mathbf{k}) - \hat{b}_s^+(-\mathbf{k}) \hat{b}_s(-\mathbf{k}) \right). \quad (34)$$

In this expression  $\hat{\mathbf{r}}_{Sch}(\mathbf{k})$  is customary Schrodinger position operator  $id/d\mathbf{k}$  in momentum space when acting in single particle channel on corresponding wave function. Here we remember that in general, the Dirac problem involves two group of states labeled by index  $s = 1, 2$ . The account of second pair of states will be required below while analyzing the origin of Darwin-like terms. As regards immediately ensuing discussion, this account is of no consequence and we shall omit index for the time being.

$$\hat{\mathbf{A}}(\mathbf{k}) = \mathbf{A}(\mathbf{k}) \left( \hat{a}^+(\mathbf{k}) \hat{a}(\mathbf{k}) + \hat{b}^+(-\mathbf{k}) \hat{b}(-\mathbf{k}) \right), \quad (35)$$

$$\mathbf{A}(\mathbf{k}) = -\frac{1}{2} [\mathbf{n}_z \times \nabla_{\mathbf{k}}] \ln(E_g + 2\varepsilon(\mathbf{k})). \quad (36)$$

The term  $\hat{\mathbf{B}}(\mathbf{k})$  is responsible for pair participation processes.

$$\hat{\mathbf{B}}(\mathbf{k}) = \mathbf{B}(\mathbf{k})\hat{a}^+(\mathbf{k})\hat{b}^+(-\mathbf{k}) + \mathbf{B}^*(\mathbf{k})\hat{b}(-\mathbf{k})\hat{a}(\mathbf{k}) \quad (37)$$

$$\mathbf{B}(\mathbf{k}) = \left( i \frac{\partial \Theta(\mathbf{k})}{\partial \mathbf{k}} + \frac{\sin 2\Theta(\mathbf{k})}{2} \frac{\partial \varphi(\mathbf{k})}{\partial \mathbf{k}} \right) e^{-i\varphi(\mathbf{k})} \quad (38)$$

In SQM approach the time dependence of position operator in Heisenberg representation in “free” problem is determined solely by the time dependence of creation/annihilation operators. It means that any time-dependent oscillating effects with frequency proportional to gap width, affecting single particle wave packets evolution, are due to virtual pair participation (see (37)). This result is in accord with the statement: “In terms of condensed matter physics, the Zitterbewegung is nothing but a special kind of inter-band transitions with creation of virtual electron-hole pairs” [43]. Thus in no-pair approximation, which is true at least far from scattering centers, the time-dependent self-smearing of electron is absent [44].

From (36) it follows that  $\hat{\mathbf{A}}(\mathbf{k})$  terms can be considered as due to some *rot* field which reminds Berry connection behavior. We will add always the word “like” while referring to this field as in our case it does not possess the topological properties of “real” Berry phase considered e.g. in the Bloch periodic problem [45] due to unboundedness of the spectrum in considered  $\mathbf{k} \cdot \mathbf{p}$  problem.

The projections of position operator for the first group of states into single electron channel in no-pair approximation dependent only on electron number operators are

$$\hat{x}(\mathbf{k}) = \left[ \hat{x}_{sch}(\mathbf{k}) + \frac{1}{2} \frac{\partial}{\partial k_y} \ln(E_g + 2\varepsilon(\mathbf{k})) \right] \hat{a}^+(\mathbf{k})\hat{a}(\mathbf{k}), \quad (39)$$

where  $\hat{x}_{sch}(\mathbf{k}) = i\partial/\partial k_x$ . Similarly we can write down the following expression for  $\hat{y}(\mathbf{k})$

$$\hat{y}(\mathbf{k}) = \left[ \hat{y}_{sch}(\mathbf{k}) - \frac{1}{2} \frac{\partial}{\partial k_x} \ln(E_g + 2\varepsilon(\mathbf{k})) \right] \hat{a}^+(\mathbf{k})\hat{a}(\mathbf{k}), \quad (40)$$

The coordinates in momentum representation satisfy the deformed Heisenberg algebra in single particle channel [46]

$$[\hat{x}(\mathbf{k}), \hat{y}(\mathbf{k})] = -i \frac{1}{2} \Delta \ln(E_g + 2\varepsilon(\mathbf{k})) \hat{a}^+(\mathbf{k})\hat{a}(\mathbf{k}). \quad (41)$$

This result of cause is not new. It was first postulated by Bacry [47]. In [48] this anomalous contribution to position operator in momentum space has been obtained and discussed within FW projection onto positive energy states.

For  $E_g = 0$  position operators are simplified to

$$\hat{x}(\mathbf{k}) = \left[ \hat{x}_{sch}(\mathbf{k}) + \frac{k_y}{2k^2} \right] \hat{a}^+(\mathbf{k})\hat{a}(\mathbf{k}), \quad (42)$$

$$\hat{y}(\mathbf{k}) = \left[ \hat{y}_{sch}(\mathbf{k}) - \frac{k_x}{2k^2} \right] \hat{a}^+(\mathbf{k})\hat{a}(\mathbf{k}). \quad (43)$$

Their commutator is of pure “monopole” type

$$[\hat{x}(\mathbf{k}), \hat{y}(\mathbf{k})] = -i \frac{1}{2} \delta(\mathbf{k}) \hat{a}^+(\mathbf{k})\hat{a}(\mathbf{k}). \quad (44)$$

The presented form of position operators contradict the statement that Zitterbewegung “has a close relation to Berry connection” [49]. Within proposed consideration in no-pair approximation the Berry field carrying term in defined position operators does not include the contribution of the pair creation processes and thus does not depend on time. This Berry field cannot be the origin of time-oscillation phenomenon, which is the hallmark of Zitterbewegung.

Now the idea is to replace Schrodinger operator  $\hat{r}_{Sch}(\mathbf{k}) = id/d\mathbf{k}$  in Schrodinger expression for interaction with external potential by these Berry-like phase carrying operators. To this end, we use the following chain of equalities

$$\begin{aligned} \int \frac{d\mathbf{q}}{(2\pi)^2} V(\mathbf{k} - \mathbf{q}) \varphi(\mathbf{q}) &= \int \frac{d\mathbf{Q}}{(2\pi)^2} V(-\mathbf{Q}) \varphi(\mathbf{k} + \mathbf{Q}) \\ &= \left[ \int \frac{d\mathbf{Q}}{(2\pi)^2} V(-\mathbf{Q}) e^{i\hat{\mathbf{k}}\mathbf{Q}} \right] \varphi(\mathbf{k}) \\ &= \left[ \int \frac{d\mathbf{Q}}{(2\pi)^2} V(-\mathbf{Q}) e^{-i\hat{r}_{Sch}(\mathbf{k})\mathbf{Q}} \right] \varphi(\mathbf{k}). \end{aligned} \quad (45)$$

Here  $\hat{\mathbf{k}} = -id/d\mathbf{k}$  and substitution is carried out in the last expression.

In order to simplify estimations and present the main result more clear we will again restrict ourselves to EFA. Within this approximation

$$\mathbf{A}(\mathbf{k}) \approx \frac{2\gamma^2}{E_g^2} (k_y, -k_x), \quad \mathbf{B}(\mathbf{k}) \approx \frac{\gamma}{E_g} (i, 1). \quad (46)$$

In this case the position operators commutator is

$$[\hat{x}(\mathbf{k}), \hat{y}(\mathbf{k})] = -i \frac{\gamma^2}{E_g^2} \hat{a}^+(\mathbf{k})\hat{a}(\mathbf{k}). \quad (47)$$

It is in one to one correspondence with the commutator of velocity components in the system under constant magnetic field. Now let us replace  $\hat{r}_{sch}(\mathbf{k})$  in (45) by operators  $\hat{r}(\mathbf{k})$  formed by  $\mathbf{A}(\mathbf{k})$  and  $\mathbf{B}(\mathbf{k})$ . Using frequently employed in physical problems equation

$$e^A e^B = e^{A+B+C/2}, \quad (48)$$

which is true if the commutator  $C$  of  $A$  and  $B$  commutes with both  $A$  and  $B$ . The  $\exp(-i\hat{r}(\mathbf{k})\mathbf{Q})$  can be written

as

$$e^{-i\hat{\mathbf{r}}(\mathbf{k})\mathbf{Q}} = e^{-i\frac{2\gamma^2}{E_g}k_x Q_y} e^{i\frac{2\gamma^2}{E_g}k_y Q_x} e^{i\hat{\mathbf{r}}_{Sch}(\mathbf{k})\mathbf{Q}} \\ \approx \left[1 - \frac{2\gamma^2}{E_g}(k_x Q_y - k_y Q_x)\right] e^{i\hat{\mathbf{r}}_{Sch}(\mathbf{k})\mathbf{Q}}. \quad (49)$$

It is easily verified that inserting this expression into (45) will modify external potential adding spin-orbit-type term (compare with (16)) but only this term.

The  $\mathbf{k} \cdot \mathbf{p}$  Berry phase carrying part of position operator and only it has a hand in generation of SOI-type terms in no-pair equations. Now the natural question arises: Where Darwin contribution vanishes? It is absent in presented derivation despite the fact that in the low energy regime (EFA) it is of the same order in  $\gamma k/E_g$  as spin-orbit one. In order to restore the true account for all terms of the second order we are to return to the general expression for  $\hat{\mathbf{r}}(\mathbf{k})$  (33).

In EMA the first two terms in (33) commute with pair-creating terms (37). The decomposition of  $\exp(\sum_{s=1,2} \hat{\mathbf{r}}_s(\mathbf{k})\mathbf{Q})$  up to the second order in  $\gamma k/E_g$  is based on the perturbation formula

$$e^{(a+\lambda b)t} = \sum_{n=0} \lambda^n u_n \quad (50)$$

$$u_n = \left[ \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \int_0^{t_{n-1}} dt_n b(t_1) \dots b(t_n) \right] e^{at} \quad (51)$$

$$b(t) = e^{at} b e^{-at}. \quad (52)$$

When acting in single particle channel in the first group of states, only the following contribution of the pair creation terms from the second group of states remains

$$\frac{\gamma^2}{E_g^2} \int_0^Q B_2^*(\mathbf{k}) d\mathbf{Q}_1 \int_0^{Q_1} B_2(\mathbf{k}) d\mathbf{Q}_2 = \frac{\gamma^2}{2E_g} Q^2. \quad (53)$$

Here  $\mathbf{B}_1(\mathbf{k}) = \mathbf{B}_2^*(\mathbf{k})$ . It is easy to check that addition of this term into the expression for modified potential leads to Darwin expression.

There is a striking difference in pure Dirac theory and presented consideration of semiconductor problem. It concerns the definition and “reality” of vacuum state and interpretation of downward/upward transitions in both cases [50]. In intrinsic semiconductor filled valence bands constitutes vacuum in SQM. Electrons occupy all states with negative energies and Pauli principle forbids any downward transitions. The upward transitions are interpreted as the occurrence of quasiparticle with positive mass and positive charge i.e. hole. This “hole theory” in relativistic Dirac theory has been long ago re-examined. The appropriate interpretation considers the negative Dirac continuum as charge-conjugated states of positrons with positive energy [22, 51]. Nevertheless, despite of these differences, some quasi-relativistic effects in semiconductors are of the same nature. In discussed above Darwin effect we see that while external poten-

tial contains pair creation terms involving both types of states, only those terms that are due to states which are orthogonal to considered in single particle channel participate in the effect. This is analogous to the effect considered within quantum field-theoretical simulations accompanied by analytical estimates predicting the suppression of pair production at the barrier by incoming electron due to Pauli principle[44].

The presented derivation poses the question about commonly used interpretation of spin-orbit-type and Darwin terms. In atoms, e.g., it is interpreted as electromagnetic interaction of self-induced magnetic field due to electron orbital motion with self-magnetic moment due to spin [18]. In our approach this modification can be attributed to Pauli prohibition for electrons to scatter in occupied valence states and is by construction analogous to some pseudo potential used in atomic and solid state physics. As regards Darwin term, from the point of quantum field theory it emerges because any amplitude is accompanied by the amplitude for vacuum to remain vacuum - i.e. by the bubble diagrams representing creation and subsequent annihilation of electron-hole pairs from the vacuum [52]. In considered low energy regime we restrict our consideration to single bubble approximation. The fact that Darwin term has no classical correspondence was underlined in [35].

It has been shown in [48] that position algebra becomes non-commutative after FW transformation of Dirac equation due to Berry phase contribution. In our case, the Berry connection contribution coincides with the expression obtained in [48] if no-pair assumption is valid

$$\mathbf{A}_{e,h} = -\frac{1}{2}[\mathbf{n}_z \times \nabla] \ln(E_g + 2\varepsilon(\mathbf{k})). \quad (54)$$

The corresponding Berry curvature is

$$\Omega_z = \frac{1}{2} \triangle \ln(E_g + 2\varepsilon(\mathbf{k})). \quad (55)$$

There is a difference in the role of considered  $\mathbf{k} \cdot \mathbf{p}$  Berry phase  $\Gamma_e$  and Zak Berry phase defined for the dynamics of electrons in periodic solids [45]. The latter phase is geometrical phase that characterizes the topological properties of given Bloch band. The Zak phase, gained during adiabatic motion across Brillouin zone, is an invariant. In considered problems the spectrum is unbounded. It means that in general this invariant property is lost. We can analyze instead the dependence of general expression for Berry curvature on closed path radius  $k$  and  $E_g$

$$\Gamma_e = \oint \mathbf{A}_{e,h}(\mathbf{k}) d\mathbf{k} = \int \mathbf{B}(\mathbf{k}) d\mathbf{S} \\ = 2\pi \frac{\gamma^2 k^2}{\varepsilon(k)(E_g + 2\varepsilon(k))}. \quad (56)$$

It is seen that our  $\mathbf{k} \cdot \mathbf{p}$  Berry phase exists as topological characteristic only for  $E_g = 0$ , when it does not depend on the chosen closed path radius and is equal to  $\pi$ . For

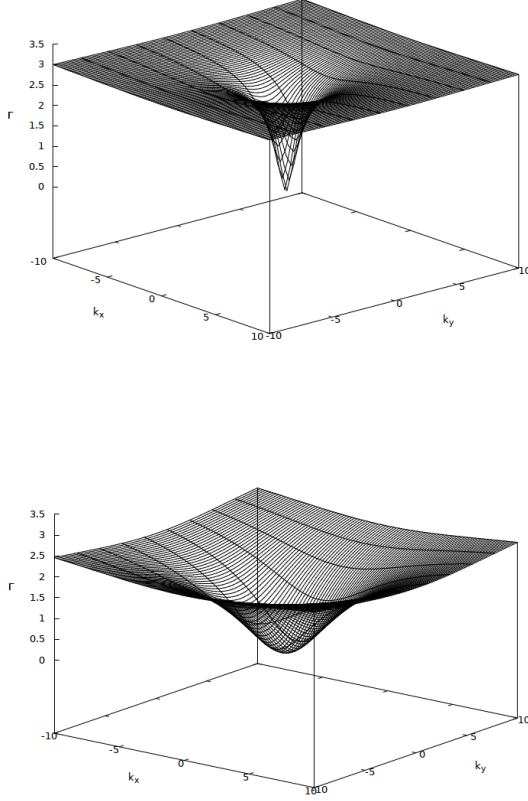


Figure 1. Dependence of Berry phase for constant radius of closed path of integration for  $E_g = 10$  mEv (top) and  $E_g = 50$  mEv (bottom),  $\gamma = 8 \cdot 10^{-8}$  mEv  $\cdot$  cm

$E_g \neq 0$  Berry phase for given contour decreases from  $\pi$  to zero with  $E_g$  increase. The dependence of Berry phase on  $k$  (radius of closed path of integration) for two different values of  $E_g$  is presented in Fig.1. In addition, the dependence of Berry phase on  $E_g$  for constant radius of contour ( $k = \text{const}$ ) is presented in Fig.2. The similar behavior of Berry phase was obtained in [53] in the tight-binding model of graphene when different on-site terms are added to the two sublattices making them nonequivalent. In our case the considered Berry phase is an “intrinsic” property of free  $\mathbf{k} \cdot \mathbf{p}$  problem. Due to the symmetry of the bands in Dirac problem all results for electrons holds for holes.

All above considerations were carried out in momentum space. Only in this representation the unambiguous separation of states carrying opposite charges is possible. The defined “no-pair” position operator (39) is local in momentum representation. It means that transformation of  $\hat{x}(\mathbf{k})$  to coordinate space makes it non-local operator  $\hat{X}$ . Its action upon electron wave function  $\psi(x, k_y)$  is

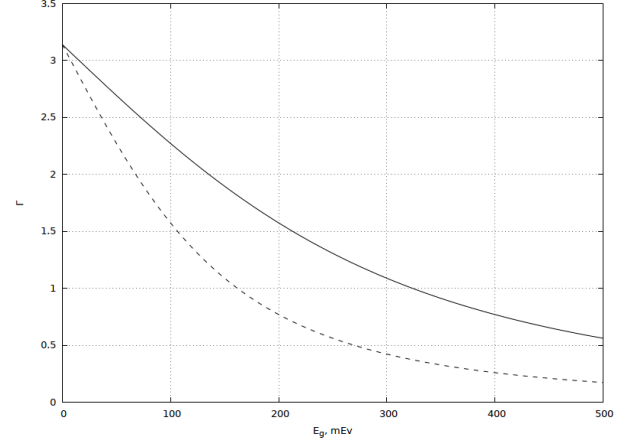


Figure 2. Dependence of Berry on  $E_g$  for constant radius of contour:  $k = 10^8 \text{cm}^{-1}$  (dashed line) and  $k = 3 \cdot 10^8 \text{cm}^{-1}$  (solid line),  $\gamma = 8 \cdot 10^{-8}$  mEv  $\cdot$  cm

defined as

$$\begin{aligned} \hat{X}\psi(x, k_y) &= \int [\hat{x}(\mathbf{k})\psi(k_x, k_y)]e^{ik_x x} dk_x \\ &= \int \int \psi(x', k_y)[\hat{x}(\mathbf{k})e^{-ik_x x'}]e^{ik_x x} dk_x dx' \\ &= x\psi(x, k_y) + \int K(x - x', k_y)\psi(x', k_y)dx'. \end{aligned}$$

The kernel  $K(x - x', k_y)$  determining non-local behavior of position operator is

$$K(\Delta x, k_y) = \frac{1}{2} \int \frac{\partial}{\partial k_y} \ln(E_g + 2\varepsilon(\mathbf{k}))e^{ik_x \Delta x} dk_x. \quad (57)$$

In the limit  $\gamma k/E_g \ll 1$  the asymptotical behavior of the kernel  $K(\Delta x, k_y)$  is

$$K(\Delta x, q_y) \sim \frac{\gamma k_y}{E_g} \left( \sqrt{2}e^{-\frac{E_g}{\sqrt{2}\gamma}|\Delta x|} - e^{-\frac{E_g}{\gamma}|\Delta x|} \right), \quad (58)$$

The smearing is determined by “Compton” wave length  $\gamma/E_g$ . In the opposite limit  $E_g \rightarrow 0$

$$K(\Delta x, k_y) \sim e^{-|k_y||\Delta x|}, \quad (59)$$

i.e. the smearing is determined by de Broglie wave length  $1/k_y$ . The non-locality of position operator was predicted for the relativistic particles in famous paper by T.D. Newton and E.P.Wigner [54]. The authors has shown that for elementary system with relativistic energy dispersion relation  $E(k) = \sqrt{E_g^2 + \gamma^2 k^2}$  the position operator becomes integral operator in position space instead of common multiplicative c-number operator. As it follows from our consideration this effect appears as long as we account for filled valence band in our multiband problem. The same effect was discussed in [3, 55, 56], where it was stated that the electrons in narrow gap semiconduc-



tors are to be considered as the extended objects of size  $\lambda \sim \hbar(m^*P)$  ( $m^*$  is the effective mass). It was pointed out that in narrow gap semiconductors  $\lambda$  can be as large as 70 Å.

#### IV. SUMMARY

The derivation of Pauli-like single-particle no-pair equations in intrinsic 2D Dirac-like semiconductors was carried out within SQM. The truncation of  $\mathbf{k} \cdot \mathbf{p}$  Hamiltonian to single particle channels leads to essential modification of external potential and lattice distortion perturbation, especially in degenerate gapless situation. We confirm the validity of proposed approach by comparison of obtained results with the well-known and experimentally established ones. The similar Pauli equations for electrons were obtained and discussed using Casimir-type positive energy projection operators [57]. We demonstrated the advantage of proposed approach over FW truncation and its variants. For example, as it has been proven in [58] the Foldy-Wouthousen transformation must be accompanied by nullification of either upper or lower components of bispinor wave function. In our approach this result immediately follows in no-pair approximation. The SQM approach presents simple and clear physical picture formulating single particle equations for both types of carriers. The difference in a role played by single particle processes and participation of virtual pairs is revealed. SQM approach allows to take

into account the effect of filled valence bands and to avoid in the cause of derivation unphysical superposition of positive and negative energy states. The account for filling modifies essentially external potential and lattice distortion perturbation entering the sought equations making them in general non-local operators. This modification does not depend on semiconductor parameters in the degenerate case and is determined by perturbation strength only. In our approach, the effective single-particle potential is constructed in such a way as to exclude scattering of electrons into occupied valence states. Remaining faithful to Pauli principle, we obtain on this way some kind of pseudo potential, which actually does not differ in essence from the one used in solid state physics. The additional insight into origin of potential modification is provided by analyzing properties of position operator in SQM. The results of [41] suggest that unobservable relativistic effects can be successfully reproduced in the systems with more “user friendly” parameters [59]. We believe that the proposed approach can serve as theoretical grounds for comparison of quasi-relativistic effects in semiconductors with numerical solutions to relativistic QFT with space-time resolution [44].

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